

Review Paper

Investigating the Mechanism of Action of SARS-CoV-2 Virus for Drug Designing



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ABSTRACT

Coronavirus Disease 2019 (COVID-19) is a viral pneumonia emerged in December 2019 in Wuhan, China. Its cause is a new virus from the coronavirus family scientifically named Coronavirus Acute Respiratory Syndrome 2 (SARS-CoV-2). In this review study, articles published in English until March 23, 2020 on new coronavirus infection were reviewed. These articles are obtained by searching in PubMed, Scopus and Google scholar databases using keywords "SARS-CoV-2", "COVID-19" and "Coronavirus". The latest COVID-19 statistics and information were extracted from the websites of World Health Organization and the Centers for Disease Control and Prevention. we investigated the effect of different compounds on the key macromolecules in promoting SARS-COV-2 infection using computational methods and bioinformatics analysis that can be considered as the best targets for designing inhibitory drugs. The most important macromolecules were Angiotensin Converting Enzyme 2 (ACE2) and Transmembrane Protease Serine 2 (TMPRSS2) receptors of the host cell surface and the structural and non-structural proteins of the virus. The most important structural protein was Spike, playing an important role in binding the virus to the ACE2 receptor of the host cell and the entry of the virus genome into it, while the key non-structural proteins were 3-Chymotrypsin-like protease (3CLpro), RNA-dependent RNA polymerase (RdRp), Papain-like cysteine proteinase (PLpro), and non-structural protein 13 (nsp13) helicase which are involved in viral genome replication and the virus' release from the host cell.

Extended Abstract

1. Introduction

Coronavirus Disease 2019 (COVID-19) is viral pneumonia that was initiated in December 2019 in Wuhan, China. The disease is caused by a new virus from the coronavirus family, which was named Severe Acute Respiratory Syndrome Coronavirus 2 (SARS-

CoV-2) by the International Commission on Taxonomy of Viruses (ICTV) on February 11, 2020. It appears to have a higher prevalence and transmission than other members of the coronavirus family, such as SARS (Severe Acute Respiratory Syndrome) and MERS (Middle East Respiratory Syndrome). However, the mortality rate of the new coronavirus is much lower than other coronaviruses. It is mainly transmitted via inhalation of respiratory droplets or secretions expelled by infected people. Fever, cough, shortness of breath, muscle pain, and fatigue are the most

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